

WHAT IS CLAIMED IS:

1. A method of identifying a WW domain binding agent, said method comprising:
- 5 (a) defining an interaction site of a WW domain based on a plurality of atomic coordinates of said WW domain;
- (b) modeling a potential binding agent that fits spatially into said interaction site;
- (c) contacting said potential binding agent with said WW domain in the presence of a WW domain substrate; and
- 10 (d) determining the ability of said potential binding agent to compete with said WW domain substrate for binding to said WW domain.
2. The method of claim 1, wherein said WW domain is a PIN1 WW domain.
3. The method of claim 1, wherein said binding agent is an agonist or antagonist of said WW domain.
- 15 4. The method of claim 1, wherein said binding agent is an inhibitory agent.
5. The method of claim 4, wherein the inhibitory agent is designed from a known inhibitor.
6. The method of claim 1, wherein said binding agent is a peptide.
- 20 7. The method of claim 6, wherein said binding agent has a sequence Tyr-pSer-Pro-Thr-pSer-Pro-Ser (SEQ ID NO:3).
8. The method of claim 1, wherein said binding agent is selected from the group consisting of a small molecule, a peptidomimetic, and an antibody.
9. The method of claim 1, wherein said binding agent is selected by providing a computer with a three-dimensional representation of said
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interaction site and using a computer algorithm to predict a three-dimensional representation of said potential binding agent.

10. The method of claim 1, wherein said plurality of atomic coordinates are as set forth in Table 1.
- 5 11. The method of claim 1, wherein said potential binding agent is designed de novo.
12. A WW domain binding agent identified by the method of claim 1.
13. A method of identifying a WW domain binding agent, said method comprising:
 - 10 (a) defining an interaction site of a WW domain based on a plurality of atomic coordinates of said WW domain;
 - (b) modeling a potential binding agent that fits spatially into said interaction site;
 - (c) 15 determining the ability of said potential binding agent to compete with a WW domain substrate for said interaction site by contacting said potential binding agent with said WW domain in the presence of said WW domain substrate.

14. A method of identifying a WW domain binding agent, said method comprising:
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- (a) modeling a potential binding agent that fits spatially into an interaction site of a WW domain defined by a plurality of atomic coordinates of said WW domain;
 - (b) contacting said potential binding agent with said WW domain in the presence of a WW domain substrate; and
 - (c) determining the ability of said potential binding agent to compete with said WW domain substrate for binding to said WW domain.
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15. A method of identifying a WW domain binding agent, said method comprising:
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- (a) modeling a potential binding agent that fits spatially into an interaction site of a WW domain defined by a plurality of atomic coordinates of said WW domain; and
 - (b) determining the ability of said potential binding agent to compete with a WW domain substrate for said interaction site by contacting said potential binding agent with said WW domain in the presence of said WW domain substrate.
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16. A method of identifying a WW domain binding agent, said method comprising:
- determining the ability of a potential binding agent to compete with a WW domain substrate for binding to a WW domain, wherein the potential binding agent is modeled to fit spatially into a WW domain interaction site defined by a plurality of atomic coordinates.

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27. The crystalline complex of claim 23, wherein said binding agent is a C-terminal domain of RNA polymerase II.
28. The crystalline complex of claim 23, wherein said binding agent has a sequence Tyr-pSer-Pro-Thr-pSer-Pro-Ser (SEQ ID NO:3).